

Spontaneous Symmetry Breaking, Off-diagonal Long-range Order, and Nucleation of Quantum State

Yu Shi¹

Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel

PACS Numbers: 05.30.-d, 67.40.Db, 03.75.-b, 03.65.Bz

short title: spontaneous symmetry breaking

¹Electronic address: shiyu@aloni.cc.biu.ac.il

Abstract

Spontaneous symmetry breaking originates in quantum mechanical measurement of the relevant observable defining the physical situation, order parameter is the average of this observable. A modification is made on the random-phase postulate validating the ensemble description. Off-diagonal long-range order, macroscopic wavefunction and interference effects in many-particle systems present when there is a so-called nucleation of quantum state, which is proposed to be the origin of spontaneous gauge symmetry breaking, for which nonconservation of particle number N is not essential. The approach based on nonvanishing expectation of the field operator, $\langle \hat{\psi}(\vec{r}) \rangle$, is only a coherent-state approximation in thermodynamic limit. When $N \rightarrow \infty$, this approach is equivalent, but $\langle \hat{\psi}(\vec{r}) \rangle$ is not the macroscopic wavefunction.

1. Introduction

As a crucial concept of modern physics, spontaneous symmetry breaking (SSB) refers to that the ground state or vacuum does not possess the symmetry of the Hamiltonian. This was explained by the fact that the near-degeneracy of the ground state and the nearby excited states makes the symmetry-breaking state more stable than symmetric states against perturbation in case the physical ground state or vacuum is *not* the eigenstate of the Hamiltonian [1][2][3]. There is another case in which the physical ground state is an eigenstate of the Hamiltonian, therefore furnishes a representative of the corresponding symmetry, the typical example is the often-quoted ferromagnetism [4]. To understand why SSB occurs in this case, it seems that one usually also have to resort to a perturbation, e.g. the auxiliary magnetic field in ferromagnet, which approaches zero after the thermodynamic limit is taken. However, there can be no external field in reality. As indicated in this article, the thermodynamic limit is either not essential for SSB though it makes SSB exact in case the physical ground state is not an eigenstate of the Hamiltonian. In this article we present a general understanding of the mechanism of SSB based on basic principles of quantum mechanics, the word “spontaneous” is given a special meaning related to quantum mechanical measurement, where there is intrinsic randomness, the resort to perturbation is not needed. To our opinion, perturbation-induced symmetry breaking had better not be said to be spontaneous, though this is a semantic problem.

More discussions will be made on off-diagonal long-range order (ODLRO) and spon-

taneous gauge symmetry breaking (SGSB) . A motivation is the recent interests in Bose-Einstein condensation (BEC) renewed by the experimental realization using trapped atoms [5]. Interference of two condensates was discussed in case the number of atoms are conserved [6]. This raised some puzzles [7] regarding the previous approach to macroscopic wavefunction and spontaneous gauge symmetry breaking based on $\langle \psi(\vec{r}) \rangle \neq 0$ with the particle number N nonconserved [8][9][10][11], here $\hat{\psi}(\vec{r})$ is the field operator. We stress that $\langle \psi(\vec{r}) \rangle \neq 0$ is only an approximation, herein dubbed as “coherent state approximation” (CSA), which is a powerful approach and become exact when $N \rightarrow \infty$. The conservation of particle number is a presupposition for any isolated nonrelativistic system. When N is limited, e.g. in the BEC of “countable” atoms, CSA becomes not good. We show in this article that ODLRO, macroscopic wavefunction and SGSB emerge when there is a so-called nucleation of quantum state (NQS). SGSB occurs when the phase of the wavefunction corresponding to NQS is (relatively) determined after measurement. These notions themselves do not necessitate $\langle \psi(\vec{r}) \rangle \neq 0$. NQS directly leads to two-fluid model. Within our discussion, we introduce a new method not using the conventional ensemble description based on eigenstates of the Hamiltonian. For the interference between many-particle states to be possible, modification should be made on the random-phase postulate, which is the basis of quantum statistical mechanics. In this way, statistical mechanics is but the quantum mechanics simplified in the case of many-particle systems with no additional hypothesis. We rigorously justify the equivalence between ODLRO corresponding to a general local operator and the nonvanishingness of the coherent-state

average of this operator when $N \rightarrow \infty$, but it is shown that $\langle \psi(\vec{r}) \rangle$ is *not* the macroscopic wavefunction. The possibility of the coexistence of more than one ODLRO is also discussed from the perspective of NQS, as well as in CSA.

2. Spontaneous symmetry breaking

In this section, we explicitly give the general mechanism of SSB based on basic principles of quantum mechanics, especially, it is claimed that quantum mechanical measurement is the origin of SSB. There may be overlap or equivalence between some points here and previously known results, but all the essentials are given for completeness.

As a foundation of quantum theory, the expansion postulate states that any state of a system is a superposition of a set of eigenstates of an arbitrary observable made on it,

$$|\Psi(t)\rangle = \sum_j \Phi_j(t) |j\rangle, \quad (1)$$

where $\langle j|k\rangle = \delta_{jk}$, Φ_j is the wavefunction corresponding to $|j\rangle$. Schrödinger equation $i\hbar\partial_t|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$ reduces to $i\hbar\partial_t\Phi_j(t) = \sum_k \Phi_k(t) \langle j|\hat{H}|k\rangle$. Another basic postulate states that, after measurement, the state of the system projects, or say collapses to an eigenstate of the relevant observable, denoted as \hat{R} here. To which eigenstate the state collapses is intrinsically random though the probability is known. The physical situation is just *defined* by this relevant observable rather than by the Hamiltonian, though the latter governs the evolution of the state. So the physical ground state, i.e. the state with least energy which can be reached in the given situation, must be an eigenstate of the

relevant observable \hat{R} , hence may not be the ground state of the Hamiltonian \hat{H} . Choose $|j\rangle$ in (1) be the eigenstate of \hat{R} . If \hat{R} commutes \hat{H} , they have common eigenstates, $|j\rangle$ is also the eigenstate of \hat{H} , then $\langle j|\hat{H}|k\rangle = E_j\delta_{jk}$, $\Phi_j(t) = a_j e^{-iE_j t/\hbar}$, where a_j is independent of time. If at time $t = 0$, the state is in an eigenstate $|I\rangle$, then $|\Psi(t)\rangle = e^{-iE_I t/\hbar}|I\rangle$, i.e. the system is always in $|I\rangle$. Therefore after measurement the state of system must be trapped in a stationary state and the physical ground state is just the ground state of \hat{H} . If there is degeneracy, i.e. there are more than one stationary state corresponding to an eigenvalue of \hat{R} and \hat{H} , these states form a (non-identical) representation of the relevant group, the above mechanism just gives rise to one type of SSB, herein referred to as type-1 SSB. It may be seen that it is just the symmetry of \hat{H} that keeps the spontaneous breaking of this symmetry.

If \hat{R} is not commutative with \hat{H} , then generally $\langle j|\hat{H}|k\rangle \neq 0$ even for $k \neq j$, therefore $\Phi_j(t) \neq 0$ for any j even if $\Phi_j(t=0) = \delta_{jI}$. This means that the state of the system cannot be trapped in an eigenstate of \hat{R} though it is an eigenstate of \hat{R} just after measurement. What is interesting is that the probability $|\Phi_{j \neq I}(t)|^2$ may be very small within the observational time. Suppose the unitary transformation from the eigenstate of \hat{H} , say $|j'\rangle$, to that of \hat{R} , say $|j\rangle$, is $|j\rangle = \sum_{j'} U_{jj'} |j'\rangle$. If $|\Psi(t=0)\rangle = |j\rangle$, then $|\Psi(t)\rangle = \sum_{j'} U_{jj'} e^{-iE_{j'} t/\hbar} |j'\rangle$, the probability for the state to be in the eigenstate $|k\rangle$ of \hat{R} is then $|\langle k|\hat{\Psi}(t)\rangle|^2 = |\sum_{j'} U_{kj'}^* U_{jj'} e^{-iE_{j'} t/\hbar}|^2$, which is near to δ_{kj} if $E_{j'}$ is near to each other. Particularly, for a two-state system, if $|\Psi(t=0)\rangle = |1\rangle$, then $|\langle 2|\hat{\Psi}(t)\rangle|^2 \propto \sin^2[(E'_1 - E'_2)t/2\hbar]$. Here $|1\rangle$ and $|2\rangle$ are the two eigenstates of \hat{R} .

For instance, in an ammonia molecule \hat{R} is the position operator of the nitrogen atom. For the massive neutrino, \hat{R} corresponds the generation and distinguishes ν_e , ν_μ or ν_τ , this mechanism gives rise to the neutrino oscillation, which however, must be very slow. So if the eigenstate of \hat{R} is superposed by near-degenerate eigenstates of H , there can be an effective SSB, referred to as type-2 SSB. Unlike type-1, type-2 SSB is not absolute, it is valid compared with the observational time and may be exact for infinitely large system, or say in thermodynamic limit. Now there is no common set of eigenstates of \hat{R} and \hat{H} , the physical ground state must be a superposition of the ground state and nearby excited states of \hat{H} . SSB occurs whenever a measurement is performed in case there is a symmetry corresponding to the same eigenvalue of \hat{R} under the condition of degeneracy or near-degeneracy, so in principle it is not restricted to ground state. When the eigenvalue of \hat{R} is zero, the symmetry is not broken. We also note that in the case without symmetry, the same mechanism may lead to spontaneous ergodicity breaking. Our classification here is consistent with that of Peirls [2], but he attribute the type-two here to perturbations while no explanation was made on type-1, so there are essential differences. We expose that it is the the projection of quantum mechanical measurement that originats the result that the physical state, usually the ground state, is in one of the eigenstates, which are related to each other by symmetry, rather than in a superposition which possess symmetry explicitly. The degeneracy or near-degeneracy is a guarantee of this result. In this way, as an essential element of SSB, spontaneousness can be thought to be related to the intrinsic quantum mechanical randomness, i.e. one cannot predict to which eigenstate of \hat{R} the

system collapses in a single run of measurement. The symmetry breaking in classical systems is simply induced by a perturbation, and there is no possibility of superposition at all, so we suggest it had better not be said to be spontaneous.

Let us examine the prototype of type-1 SSB, the ferromagnetism (FM). $\hat{H} = \sum_{(ij)} J_{ij}(S_i^z S_j^z + S_i^+ S_j^-)$ with $J_{ij} < 0$, $S_i^\pm = S_i^x \pm iS_i^y$. In this case of isotropy and without magnetic field, it should be stressed that *z direction is only determined after measurement*. $\hat{R} = \sum_i S_i^z$. $[\hat{H}, S_i^z] = 0$ and thus $[\hat{H}, \hat{R}] = 0$, so the physical ground state is just the ground state of \hat{H} , and is also an eigenstate of S_i^z . Since $S_i^\pm |S_i^z > = \sqrt{S(S+1) - S_z(S_z \pm 1)} |S_i^z \pm 1 >$, the contribution of second term of \hat{H} always gives zero. Thus in ground state all S_i^z have the largest eigenvalue S to make the eigenvalue of \hat{H} lowest. The ground state is degenerate with $SO(3)$ symmetry, meaning that z direction is arbitrary. But it is determined after measurement, which direction is determined to be z direction is random. Whenever it is determined, it is kept forever. The usual method of applying an infinitesimal magnetic field is a practical way of calculation but can not serve as an explanation for SSB in quantum system, though there is no problem for classical Ising model [12]. If there is an easy axis, there is no symmetry to break. If there is an easy plane, there is an $SO(2)$ symmetry to be spontaneously broken after measurement. SSB at a finite temperature refers to that the magnetization with non-zero but not the largest value spontaneously select a direction after measurement. Therefore resorting to the project postulate of quantum mechanical measurement, we understand that *spontaneous magnetization can occur without external magnetic field*.

Type-2 SSB is exhibited in systems with two or more alternative states with a non-zero transition probability between each other, e.g. molecules such as hydrogen, ammonia and sugar, as well as K -meson and the possible massive neutrino, etc. For antiferromagnetism (AFM) on a bipartite lattice, $\hat{R} = \sum_i S_i^z - \sum_j S_j^z$, where i, j belong to two sublattices, respectively. $[\hat{H}, \hat{R}] \neq 0$, so SSB in AFM is type-2, the physical ground state must be a combination of the ground state and the nearby excited states of \hat{H} . This is supported by the fact that Neel state is not an eigenstate of \hat{H} , and by that there are excitations proportional to $1/N$ [13][2]. The near-degeneracy in AFM and its difference with FM was emphasized [4].

3. Random-phase postulate and interference between many-particle states

Consider interference between two states $|\Psi(a)\rangle$ and $|\Psi(b)\rangle$, one obtains from (1) that $\langle \Psi(a) | \Psi(b) \rangle = \sum_j |\Phi_j(a)|^* |\Phi_j(b)| e^{i[\phi_j(b) - \phi_j(a)]}$, where ϕ_j is the phase of Φ_j . As the basis of quantum statistical mechanics, the random phase postulate states that the time average of $\Phi_i^* \Phi_j$ vanishes for $i \neq j$ over an interval short compared to the resolving time of observation but long compared to molecular time, therefore the system can be described as an incoherent superposition of stationary state [11]. The average of quantity \hat{O} , $\langle \Psi | \hat{O} | \Psi \rangle = \sum_{ij} \Phi_i^* \Phi_j \langle i | \hat{O} | j \rangle$ consequently reduces to $\sum_i \rho_i \langle i | \hat{O} | i \rangle$, ρ_i make up the density matrix, which is diagonal. In some textbooks [14], the diagonalization of density

matrix is approached by arguing that there is always a certain representation where the density matrix is diagonal. This is insufficient, since it is uncertain that this representation is that of Hamiltonian. Thus the random-phase postulate is necessary to make the density matrix diagonal in every representation, therefore in that of Hamiltonian. However, for the time average of $\Phi_i^* \Phi_j$ to vanish, each phase must randomly change with time. Therefore the system cannot be isolated [11], but on the contrary the result is actually applied to isolated systems. Another unsatisfactory point is that an additional time average is made on the quantum mechanical average. But in fact the element of time average has been contained in quantum mechanical average. Furthermore, *this postulate implies that there cannot be interference among many-states systems*, since the time average of each term in $\langle \Psi(a) | \Psi(b) \rangle$ would vanish under this assumption. Therefore the assumption that each phase change with time has actually been falsified by Josephson effect and will by other interference effects in many-body systems such as Bose condensates. Here we modify the random phase postulate to that *each phase ϕ_j is random and unpredictable but does not change with time and is determined after measurement*. Of course only relative values are meaningful for phases. The assumption that the phases are random at each time was made in the derivation of the master equation [15], however, to our knowledge, there was no attempt in assuming that they do not change with time. The randomness and unpredictability is consistent with the gauge symmetry, the determination of the phase is just SGSB. This modification is actually a supplement to the expansion postulate, its validity is independent of the particle number. Many-body effect exhibits in that when

the number of eigenstates $\rightarrow \infty$, $\Phi_i^* \Phi_j < i | \hat{O} | j >$ with $i \neq j$ cancel each other since the differences of phases are consequently also random, thus the ensemble description is validated though generally $\Phi_i^* \Phi_j$ does not vanish. Hence the ensemble average or say thermodynamic average is just the quantum mechanical average reduced under the many-body effects, hereafter we only use the term “average”. That the ensemble average equals long-time average is thus not an additional hypothesis of statistical mechanics, but because they are both quantum mechanical average by definition. Therefore statistical mechanics is nothing but a special case of quantum mechanics without additional hypotheses.

Normally the interference $< \Psi(a) | \Psi(b) >$ vanishes when the number of eigenstates $\rightarrow \infty$. But it is interesting that interference effect emerges when there is a dominant one among $|\Phi_j(a)| |\Phi_j(b)|$, i.e. if $|\Phi_1(a)|$ and $|\Phi_1(b)|$ corresponding to an eigenstate $|1 >$ are finite fractions so that $\Phi_1^*(a) \Phi_1(b)$ cannot be cancelled. In this case, however, the simplification of $< \Psi | \hat{O} | \Psi >$ is not affected, since $\Phi_i \Phi_j$ here is of the same system, the phase difference in each off-diagonal terms is random but that in each diagonal term is zero. Therefore our modification is quite reasonable.

4. Nucleation of quantum state, off-diagonal long-range order and spontaneous gauge symmetry breaking

We have seen that to allow the possibility of interference between many-particle states, there should exist an eigenstate, say $|1\rangle$ with $\Phi_1 = \sqrt{\alpha}e^{i\phi_1}$ while $|\Phi_j| \ll |\Phi_1|$ for $j \neq 1$. α denotes a finite fraction hereafter. This situation may be termed as “nucleation of quantum state” (NQS). The physics of NQS is nothing beyond BEC or ODLRO in general. However, NQS can serve as a useful notion regarding the whole system, while BEC regards constituent particles. Note that the physical situation is defined by the relevant observable, so when we discuss actual happening NQS, it is most convenient to choose the set of eigenstates to be that of the relevant observable. Therefore we know that the eigenstate should be stationary or nearly stationary for effects of NQS to exhibit. This is just the condition of SSB. Actually here it is gauge symmetry that is spontaneously broken, reflected in that the phase of the wavefunction of the eigenstate to which the state nucleates is random and determined by measurement.

BEC occurs when there is a finite density of particles in the zero-momentum state. Generally it can be characterized by ODLRO, i.e. the nonvanishingness of one-particle reduced density matrix $\langle \vec{r}' | \hat{\rho}_1 | \vec{r} \rangle = \langle \hat{\psi}^\dagger(\vec{r}') \hat{\psi}(\vec{r}) \rangle$ [16] [17], which can be factorized as

[17][9]

$$\langle \hat{\psi}^\dagger(\vec{r}') \hat{\psi}(\vec{r}) \rangle = \sum_n \lambda_n f_n^*(\vec{r}') f_n(\vec{r}), \quad (2)$$

where $f_n(r)$ is the eigenfunction of $\hat{\rho}_1$ with eigenvalue λ_n . ODLRO is equivalent to the existence of $\lambda_1 = N\alpha$. This concept is general for reduced density matrices $\hat{\rho}_n$ and provides a unified framework for superfluidity and superconductivity [17]. It was later thought that the main part of (2) is just $\langle \hat{\psi}(\vec{r}') \rangle^* \langle \hat{\psi}(\vec{r}) \rangle$, a superfluid was defined to be with nonvanishing $\langle \hat{\psi}(\vec{r}) \rangle$, which was claimed to be the macroscopic wavefunction and indicates SGSB [9]. Similar approach was adopted in BCS superconductivity (SC) [18]. A usual way of understanding $\langle \hat{\psi}(\vec{r}) \rangle \neq 0$ is to introduce an auxiliary field which is coupled to $\hat{\psi}(\vec{r})$ and approaches infinitesimal in the thermodynamic limit [11], but this field is unphysical. One may argue that it may serve mathematically as a Lagrangian multiplier for the constraint on N , but the latter has been taken into account by chemical potential. Further, as explained above, even for ferromagnetism, this method is defective and superfluous for SSB. Alternatively one may simply think that the macroscopic wavefunction of condensed particles is just $\sqrt{N_0/V} b_k$, where N_0 is number of condensed particles, b_k is the corresponding single-particle wavefunction. However, this approach reduces the phase to only that of the single-particle and thus has no physical significance [10]. Here we show that SGSB itself does not require nonconservation of particle number, the macroscopic wavefunction is derived based on NQS.

It has actually been emphasized that the conservation of particle number is necessary for BEC [11]. Viewed in our framework, the relevant observable $\hat{R} = \hat{N}_0$. For SC, it is

well known that BCS ground state [18] is not an eigenstate of either \hat{H} or \hat{N} . However, since the electron number is conserved, BCS ground state is only an approximation for convenient calculation [18]. There is still no exact solution of BCS Hamiltonian. The real physical ground state may be conjectured to be N -particle projection of BCS ground state, so it is $|\Psi_G\rangle \propto (\sum_k g_k \eta_k^\dagger)^{N/2} |0\rangle$, where k denotes momentum, $\eta_k^\dagger = c_{k\uparrow, -k\downarrow}$, g_k is Cooper pair wavefunction in momentum space, here N is assumed to be even. $|\Psi_G\rangle$ is of a standard form for a state with ODLRO [17], and is surely an eigenstate of \hat{H} since it is that of \hat{N} . The excited state with $N_G/2$ Cooper pairs can be given as $|\Psi_E\rangle \propto \prod_{i=1}^{N-N_G} c_{k_i}^\dagger (\sum_k g_k \eta_k^\dagger)^{N_G/2} |0\rangle$, which possesses ODLRO if $N_G = N\alpha$. This state can exist for both even and odd N . Now $\hat{R} = \hat{N}_C = \sum_k \eta_k^\dagger \eta_k$, the number of Cooper pairs, the state of the system is always its eigenstate. One may obtain $\hat{N}_C |\Psi_G\rangle = (N/2) |\Psi_G\rangle$, $\hat{N}_C |\Psi_E\rangle = (N_G/2) |\Psi_E\rangle$.

Without need of knowledge of the exact form of $|\Psi_G\rangle$ and $|\Psi_E\rangle$, the situation of SSB is known. Generally for both BEC and SC, $[\hat{H}, \hat{R}] \neq 0$, hence SSB are type-2. When all particles are condensed in BEC (paired in SC), SSB is type-1. Free bosons always satisfy $[\hat{H}, \hat{N}_0] = 0$, hence SSB would always be type-1, but since the number of particles in each momentum state is conserved, BEC cannot occur unless it is prepared at the beginning.

Now we show NQS gives rise to ODLRO, the nonvanishing term in ODLRO function is factorized by a macroscopic wavefunction for a system with conserved number of particles.

Not reduced to the conventional ensemble description using eigenstates of \hat{H} , the one-

particle ODLRO function is just $\langle \Psi | \hat{\psi}^\dagger(\vec{r}') \hat{\psi}(\vec{r}) | \Psi \rangle$. Now we expand $|\Psi\rangle$ by the eigenstate of the relevant observable \hat{R} . Let $\hat{R} = \hat{N}_{k_0}$, the number of particles with momentum k_0 , the eigenstates correspond to various values of N_{k_0} . Suppose NQS occurs in the eigenstate $|1\rangle$ where all N particles occupies k_0 single-particle state. Therefore the ODLRO function is

$$\begin{aligned}
\langle \Psi | \hat{\psi}(\vec{r}')^\dagger \hat{\psi}(\vec{r}) | \Psi \rangle &= \frac{1}{V} \sum_{kk'} \langle \Psi | a_{k'}^\dagger a_k | \Psi \rangle b_{k'}^*(\vec{r}') b_k(\vec{r}) \\
&= \frac{1}{V} \sum_j \Phi_j^* \Phi_j \sum_k \langle j | a_k^\dagger a_k | j \rangle b_k^*(\vec{r}') b_k(\vec{r}) + \text{small terms} \\
&= \frac{N}{V} \Phi_1^* \Phi_1 b_{k_0}^*(\vec{r}') b_{k_0}(\vec{r}) + \text{small terms} \\
&= W(\vec{r}')^* W(\vec{r}) + \text{small terms}, \tag{3}
\end{aligned}$$

where $W(\vec{r}) = \sqrt{N/V} \Phi_1 b_{k_0} = \sqrt{N\alpha/V} b_{k_0}(\vec{r}) e^{i\phi_1}$. So we obtain the nonvanishingness and factorization of ODLRO function to a macroscopic wavefunction $W(\vec{r})$. which is the product of the wavefunction of the whole system and that of a single particle giving position dependence within the system. In this way we get a phase ϕ_1 in addition to that of the single-particle wavefunction. $\int W^*(\vec{r}) W(\vec{r}) d\vec{r} = N \Phi_1^* \Phi_1$. In principle, BEC can happen for a non-zero k_0 , but the free energy should be made to be a minimum. Many discussions are based on a macroscopic wavefunction, with the identification as $\langle \hat{\psi} \rangle$ only serve as an irrelevant interpretation. Now it is derived from NQS.

For fermion systems, there cannot be NQS in single-particle states constrained by Pauli principle, but it can occur in two- or even-number-particle states. This is consistent with that the relevant observable in SC is pair operator. In this case, $|\Psi\rangle$ is expanded in

two-particle states. NQS refers to that there is a nonvanishing probability for all particles occupy a particular two-particle state. Factorization of ODLRO function can be obtained in a way similar to (3).

It is easy to see that NQS in n -particle states corresponds to the existence of ODLRO for n -particle states, i.e. that of eigenvalues of the order N for n -particle reduced density matrix [17]. Various statements corresponding to ODLRO [17] can be made. For example, the smallest n for which NQS occurs gives the collection of n particles which form a basic group exhibiting the long-range order. NQS in n -particle state implies that in m -particle states for $m \geq n$. If the probability of all particles occupying a single-particle state is α , then the probability that all two-particle pairs occupy the two-particle state formed by that single-particle state is obviously α^2 .

NQS directly leads to two-fluid model [19][20] [21][11] and proves its universality. The density is $\langle \Psi | \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) | \Psi \rangle$ while the current is $2\hbar/m \cdot \text{Im}(\langle \Psi | \hat{\psi}^\dagger(\vec{r}) \vec{\nabla} \hat{\psi}(\vec{r}) | \Psi \rangle)$, where $\hat{\psi}(\vec{r})$ is replaced by a pair of electron operator for SC. So the density and current of the superfluid component are $|W(\vec{r})|^2$ and $2\hbar/m \cdot \text{Im}(W^* \vec{\nabla} W)$, respectively. The rest terms describe normal-fluid component. Decomposition of free energy is more complicated, as indicated by Gorter-Casimir model [20].

NQS implies that *the precise meaning of BEC is that the probability that all particles are in a particular momentum state is a nonvanishing α* , with an objectively random phase, which however does not change with time. SGSB occurs when this phase is measured. In conventional ensemble description only the average of N_k is given since it is

not a conserved quantity. The only exception is that N_{k_0} is conserved when $N_{k_0} = N$, but in this case $\alpha = 1$ and thus the probability for all particles occupy k_0 state is unity. So there is no contradiction between the present and the conventional viewpoints. When the probability for the state of a system to be in an eigenstate is unity, there is still an objectively random phase to be determined after measurement. Of course, only relative phase is meaningful. NQS is necessary for SGSB, their existence is independent of whether the particle number is conserved. A free particle, for example, is always in the state of NQS with probability unity, SSB of gauge symmetry occurs when its (relative) phase is measured. NQS may possibly exist in spaces other than momentum space, it is interesting to explore BEC in real space to make an ultra-dense object, possessing ODLRO in momentum space.

Certainly it is possible that NQS occurs in two or more eigenstates or non-orthogonal states, This is usual for few-particle systems. For many-particle systems, this naturally leads to the coexistence of more than one ODLRO. This possible situation was first considered in [22] for Cooper-paired states with nonzero angular momentum, and was disfavored in [9]. Recently there are more interests in this topic, as for example in [23][24][25][26].

5. Order parameter

We have seen that SSB widely exists, not limited to phase transition. Phase transition gives rise to symmetry breaking. For classical system, it is induced by a perturbation which may be very small. For quantum system it is SSB. Since the physical situation is just defined by the relevant observable, the symmetry breaking is reflected in the change of its value. This applies also for non-spontaneous symmetry breaking. Naturally, order parameter, which designates the change of symmetry, is just the average of \hat{R} , e.g. that of FM phase transition is the magnetization. The mass of liquid can serve as that for gas-to-liquid transition, NQS is just its quantum correspondence, the order parameter is obviously the probability of nucleating to the particular eigenstate. Thus *the order parameter of BEC (SC) is the fraction of condensed (paired) particles*, and is therefore equivalent to the magnitude of the macroscopic wavefunction and thus does not contradict Ginzburg-Landau theory, it is also proportional to the nonvanishing term in ODLRO function. Not only for phase transition, either not only for SSB, order parameters can also be defined for other symmetry breakings. Thermodynamic limit is necessary for phase transitions, but may be unnecessary for other SSB though it makes type-2 SSB exact.

6. Coherent-state approximation

It is well known that the coherent state $|\Psi_c\rangle$ is formed by states with different number of particles N , say $|\Psi_N\rangle$,

$$|\Psi_c\rangle = \sum_N f_N |\Psi_N\rangle, \quad (4)$$

where the coefficients f_N and thus the weights in expectation values center around the mean value of N , say $\langle N \rangle$, with a spread of $\sim \sqrt{\langle N \rangle}$ [9][18][2]. Therefore CSA is quite similar to the grand canonical ensemble approach. We have shown that coherent state is not essential for SGSB. However, CSA is a convenient approach which becomes exact when $N \rightarrow \infty$.

The concept of ODLRO can be generalized to other local operator, denoted as $\hat{B}(\vec{r})$.

For a N -particle system, the long-range order of $\hat{B}(\vec{r})$ exists if and only if $\langle \Psi_N | \hat{B}^\dagger(\vec{r}') \hat{B}(\vec{r}) | \Psi_N \rangle \rightarrow \rho\alpha$ as $|\vec{r} - \vec{r}'| \rightarrow \infty$, here ρ is the density N/V , which is kept constant for different N . In this section we establish the equivalence between ODLRO in a system with a conserved number of particles and the nonvanishingness of coherent-state expectation of the corresponding operator, e.g. the field operator $\hat{\psi}(\vec{r})$.

Consider the ODLRO function for coherent state $|\Psi_c\rangle$,

$$\begin{aligned} \langle \Psi_c | \hat{B}^\dagger(\vec{r}') \hat{B}(\vec{r}) | \Psi_c \rangle &= \sum_N |f_N|^2 \langle \Psi_N | \hat{B}^\dagger(\vec{r}') \hat{B}(\vec{r}) | \Psi_N \rangle \\ &= \rho\alpha \end{aligned} \quad (5)$$

In the derivation, we used the property that $\hat{B}^\dagger(\vec{r}') \hat{B}(\vec{r})$ conserve the particle number. Thus there is ODLRO in $|\Psi_c\rangle$ if and only if there is ODLRO in $|\Psi_N\rangle$. Then the

key point is the factorization of $\langle \Psi_c | \hat{B}^\dagger(\vec{r}') \hat{B}(\vec{r}) | \Psi_c \rangle$, which has been widely taken for granted.

Note that $|\Psi_c\rangle$ is not the reality but a subjective construction with infinite terms. Therefore one can always find a set of f_N so that $|\Psi_c\rangle$ is an eigen-vector of $\hat{B}(\vec{r})$. Furthermore, $|\Psi_c\rangle$ can be an eigenstate of *any* local operator since there are infinite f_N -s. Hence

$$\begin{aligned} \langle \Psi_c | \hat{B}^\dagger(\vec{r}') \hat{B}(\vec{r}) | \Psi_c \rangle &= \sum_{\beta} \langle \Psi_c | \hat{B}^\dagger(\vec{r}') | \beta \rangle \langle \beta | \hat{B}(\vec{r}) | \Psi_c \rangle \\ &= \langle \Psi_c | \hat{B}^\dagger(\vec{r}') | \Psi_c \rangle \langle \Psi_c | \hat{B}(\vec{r}) | \Psi_c \rangle, \end{aligned} \quad (6)$$

where $\{|\beta\rangle\}$ is the complet set of eigenstates to which $|\Psi_c\rangle$ belongs.

Therefore we proved the rigorous equivalence between ODLRO and the nonvanishingness of the coherent-state expectation of the corresponding operator when $N \rightarrow \infty$. This justifies many researches concerning long-range orders in condensed matter physics. For instance, if there exists the following commutation relation

$$[\hat{H}_N, \hat{A}(\vec{r})] = \gamma_B B(\vec{r}) + \gamma_C C(\vec{r}), \quad (7)$$

where \hat{H}_N is the Hamiltonian of N -particle system, $\hat{A}(\vec{r})$, $B(\vec{r})$ and $C(\vec{r})$ are local operators, γ_B and γ_C are complex constants, one may claim that the long-range orders of $B(\vec{r})$ and $C(\vec{r})$ must be either present or absent simultaneously. In particular, if there is only one local operator appears on the right-hand side of (7), its long-range order must be absent. This conclusion can be obtained simply by calculating the coherent-state expectation of (7) and noting that of the left-hand side vanishes. This method was applied

to obtain constraints on pairings within the Hubbard model [23][24]. However, it was argued that this approach is not rigorous since the eigenvalue of the Hamiltonian for an infinite system is ill-defined, alternative theorems were given regarding N -particle system [25]. Through the above justification, it is clear that these two approaches are rigorously equivalent when $N \rightarrow \infty$. Especially, the property of $|\Psi_c\rangle$ that it is an eigenstate of any local operator is crucial in obtaining the simultaneous nonvanishingness of the expectation values of $B(\vec{r})$ and $C(\vec{r})$ generally. Because it is the coherent-state $|\Psi_c\rangle$ that of which the expectation is calculating for (7), and $|\Psi_c\rangle$ is a superposition of $|\Psi_N\rangle$ with different values of N , only eigenvalue of \hat{H}_N with different values of N are dealt with in obtaining the coherent-state expectation of (7), the problem of ill-definition is eliminated.

It is easy to see that NQS in the state with the particle number conserved is equivalent to NQS in the coherent state, since the expansion structure (1) of $|\Psi_N\rangle$ in (4) is the same for different values of N . The macroscopic function in CSA remains the same as the original one, given $\rho = N/V$ is constant for different N .

When $N \rightarrow \infty$, $|\Psi_c\rangle \rightarrow f_{<N>}|\Psi_{<N>}\rangle$. Since $\hat{\psi}(\vec{r}) = (1/\sqrt{V}) \sum_k \hat{a}_k b_k(\vec{r})$, $\hat{\psi}(\vec{r})|\Psi_{<N>}\rangle = \sqrt{\langle N \rangle / V} b_{k_0} \Phi_1 |1\rangle_{<N>-1} + \text{small terms}$, where k_0 denotes the single-particle state into which particles condense, $|1\rangle_N$ is the state in which NQS occurs for N -particle system. It is difficult to evaluate the exact form of $\langle \hat{\psi}(\vec{r}) \rangle$, since $\hat{\psi}(\vec{r})$ changes the number of particles thus the sum of the small terms is possibly non-negligible. But it is clear that only $\Phi_i^* \Phi_j$ instead of Φ_i appears in each term. Compared with the macroscopic wavefunction $W(\vec{r}) = \sqrt{\rho} \Phi_1 b_{k_0}$, $\langle \hat{\psi}(\vec{r}) \rangle$ is certainly *not* equal to the macroscopic wavefunction,

though it can serve as a convenient characteristic of NQS and long-range order.

7. Summary

To summarize, SSB originates in quantum mechanical measurement of the relevant observable defining the physical situation, and may be classified to two types according to whether this observable commutes the Hamiltonian. Order parameter may be generally defined as the average of this relevant observable. To allow the possibility of the interference between many-particle systems, we modify the random phase postulate, which is the basis of quantum statistical mechanics. The phase of the wavefunction corresponding to each eigenstate is random and unpredictable but does not change with time. This statement is actually a supplement to expansion postulate of quantum mechanics. Thus statistical mechanics is but a special case of quantum mechanics with no additional hypotheses, incoherent ensemble description is a natural consequence of many-body effects. Interference between many-particle systems, ODLRO and macroscopic wavefunction are derived from nucleation of quantum state. Spontaneous gauge symmetry breaking occurs when the phase of macroscopic wavefunction is determined (relatively) after measurement. Since quantum mechanical measurement is still an open problem, whether SSB is a dynamical process within a finite time or a discontinuous process is beyond the scope of present work. Clarification of this issue is in no doubt of great importance.

Nonconservation of particle number is not essential for SGSB. The coherent-state

approach is an approximation which may become exact when $N \rightarrow \infty$. Although the nonvanishing $\langle \hat{\psi}(\vec{r}) \rangle$ under CSA can serve as a characteristic of long-range order, it is *not* the macroscopic wavefunction.

Theories of spontaneous gauge symmetry breaking in relativistic field theory are based on assuming the nonvanishingness of vacuum expectation of a scalar field. This conflicts the basic fact that the Hilbert space is spanned by states with definite number of particles and/or antiparticles in each mode. We made an attempt to modify these theories to eliminate the assumption that the vacuum expectation of the scalar field is nonvanishing. [27].

The present work also reminds that there is no classical-quantum boundary, principles of quantum mechanics apply in all scales. “Classicality” is an emergent property of systems with many degrees of freedom in the absence of NQS. The macroscopic quantum effect in superconductivity and superfluidity first proposed by London [21] is a consequence of NQS.

References

- [1] In this article, “physical ground state” means the state with the least energy among those accessible in the given physical situation, while “ground state of the Hamiltonian” refers the eigenstate of the Hamiltonian with the least eigenvalue
- [2] Peirls R 1991 *J. Phys. A* **24** 5273; 1992 *Contemporary Phys.* **33** 221
- [3] Weinberg S 1996 *Quantum Theory of Fields* Vol. II (Cambridge: Cambridge University)
- [4] One may claim this case not be SSB, see, e.g., Anderson P W 1990 *Phys. Today* 117, however, as commented in [2], this is problem of semantics, but it would be inconvenient not to include this important case. Actually most literature quote ferromagnet as the introductory example of SSB. The present article show the common origin of this case and the case in which the physical ground state is not an eigenstate of the Hamiltonian
- [5] Anderson M H *et al.* 1995 *Science* **269** 198; Bradley C C *et al.* 1995 *Phys. Rev. Lett.* **75** 1687; Davis K B *et al.* 1995 *ibid.* **75** 3969
- [6] Juvanainen J and Yoo S M 1996 *Phys. Rev. Lett.* **76** 161; Naraschewski M *et al.* 1996 *Phys. Rev. A* **54** 2185; Cirac J I *et al.* 1996 *Phys. Rev. A* **54** R3714; Wong T *et al.* 1996 *Phys. Rev. A* **54** R3718

- [7] See, e.g., Lalöe F 1996 *Europhysics News* **27** 174
- [8] Goldstone J 1961 *Nuovo Cim.* **19** 154.
- [9] Anderson P W 1966 *Rev. Mod. Phys.* **38** 298.
- [10] Leggett A J and Sols F 1991 *Found. Phys.* **21** 353; Leggett A J 1995 *Bose-Einstein Condensation* ed A Griffin, D W Snoke and S Stringari (Cambridge: Cambridge University)
- [11] Huang K 1987 *Statistical Mechanics* (New York: John Wiley & Sons)
- [12] Yang C N 1952 *Phys. Rev.* **85** 809
- [13] Anderson P W 1951 *Phys. Rev.* **80** 694
- [14] See, e.g., Feynman R P 1972 *Statistical Mechanics* (Reading: Benjamin)
- [15] Van Hove L 1962 *Fundamental Problems in Statistical Mechanics* ed E G D Cohen (Amsterdam: North-Holland)
- [16] Penrose O 1951 *Phil. Mag.* **42** 1373; Penrose O and Onsager L 1956 *Phys. Rev.* **104** 576
- [17] Yang C N 1962 *Rev. Mod. Phys.* **34** 694
- [18] Bardeen J, Cooper L N and Schrieffer J R, *Phys. Rev.* 1957 **108** 1175; Schrieffer J R 1964 *Theory of Superconductivity* (New York: Benjamin)

- [19] Tisza L 1938 *Nature* **141** 913; 1947 *Phys. Rev.* **72** 838
- [20] Gorter G J and Casimir H G B 1934 *Z. Phys.* **35**, 963
- [21] London F 1950 *Superfluids* Vol. 1 (New York: John Wiley & Sons); 1954 *ibid*
Vol. 2 (New York: John Wiley & Sons)
- [22] Gor'kov L P and Galitskii V M 1961 *Soviet Phys.-JETP* **13** 792
- [23] Zhang S C 1990 *Phys. Rev. B* **42** 1012
- [24] Shi Y 1995 *Phys. Rev. B* **51** 16619
- [25] Tian G S 1993 *J. Phys. A: Math. Gen.* **26** 2325; 1997 *ibid.* **30** 841
- [26] Shi Y *Commun. Theor. Phys.* to be published; 1997 *LANL Report-No.* cond-mat/9703009
- [27] Shi Y 1997 *LANL Report-No.* hep-th/9703013